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Chemically engineered multiferroic Morphotropic Phase Boundary in $BiFeO_3$-based single phase multiferroics

J. Zhuang[1*], A.A. Bokov[2,1], N. Zhang[1], J. Zhang[1], W. Ren[1], Z.-G. Ye[2,1]

[1]*Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University, 710049, Xi'an, P. R. China*
jzhuang@xjtu.edu.cn

[2]*Department of Chemistry and 4D LABS, Simon Fraser University, V5A 1S6, Burnaby, Canada*

As the reach points of different phases with complex structural features, morphotropic phase boundary (MPB) in ferroelectric and ferromagnetic solid solutions can significantly enhance the piezoelectric performance and magnetostrictive response, respectively. Recently, the phase-change functional responses related to the multiferroic MPB are proposed to be a promising way to enhance the magnetoelectric coupling in $BiFeO_3$-based single phase multiferroics [1]. In this work, we verify the tunable magnetic ordering and the construction of multiferroic MPB by engineering the chemical concentrations of the ferroelectric $PbTiO_3$ or magnetic $DyFeO_3$ end member in the $BiFeO_3$-$DyFeO_3$-$PbTiO_3$ ternary solid solution system. Based on the results obtained in our lab [2-3] and reported in the literature [4-6], the structure-ferroic properties phase diagram of $BiFeO_3$-$DyFeO_3$-$PbTiO_3$ ternary system is established (see Fig. 1), where a compositional region with coexisting ferroelectric polarization and ferromagnetic moment is found. More importantly, a multiferroic MPB line separating two chemical regions with distinct crystal structures and ferroic orderings is discovered in the phase diagram. The phase changing nature of MPB compositions with temperature and compositions are investigated from room temperature to high temperature paraelectric phase. This work could provide a promising system to explore the highly desired colossal effects on magnetoelectric coupling in single phase multiferroics by phase-change functional responses.

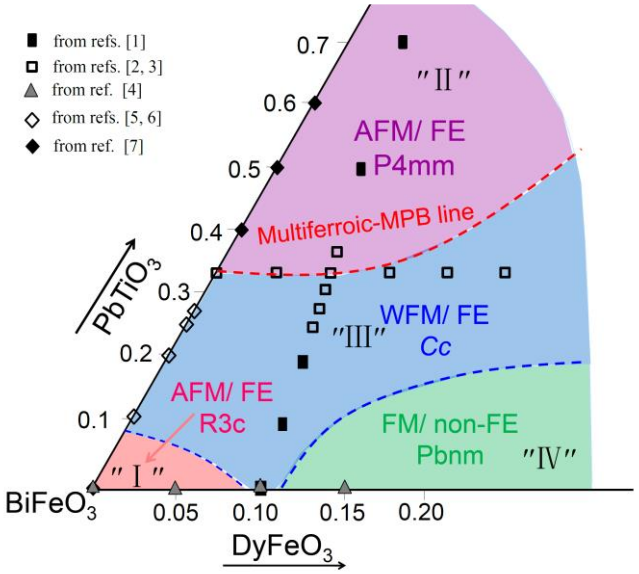

Figure 1. The sketched structure-ferroic properties phase diagram of the $BiFeO_3$-$DyFeO_3$-$PbTiO_3$ ternary system, indicating the following phase regions: FE = Ferroelectric Phase, non-FE = Non-ferroelectric Phase, FM = Ferromagnetic or Ferromagnetic Phase, AFM = Antiferromagnetic Phase, and showing a multiferroic-MPB line.

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